数学与系统科学研究院

计算数学所学术报告

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报告题目：

Geometric flow for biomolecular solvation

邀请人： 卢本卓 研究员

报告时间：**2013** 年 **5** 月 **16** 日（周四）

下午 **16:00-17:00**

报告地点： 科技综合楼三层 **311**

计算数学所报告厅

Abstract:

Solvation is a key component for understanding the structure, dynamics, and function of biomolecules. Both continuum-level (implicit) and molecular-level (explicit) descriptions for solvent have been used in computational models. While each level of description has its own strengths and weaknesses, implicit solvent models have become popular in many biophysical studies for their simplicity and computational efficiency, along with their reasonable accuracy. Implicit solvent models in which the polar contributions are typically decoupled from nonpolar contributions, are found to be inconsistent with recent studies on the solvation of atomistic and nanoscale solutes. Unlike most implicit solvent approaches, differential geometry-based models introduce coupling between the polar and non-polar free energy functionals through a characteristic function that describes a smooth dielectric interface profile at the solvent–solute boundary in a thermodynamically self-consistent fashion. However, such models have not been systematically parameterized and tested for their predictive power, thus limiting the use of this model. By independently varying two important parameters of the model (hydrodynamic pressure and microscopic surface tension), we studied a set of 17 small organic molecules to investigate how changes in model parameters affect the predicted solvation energies. Additionally, we investigated the effect of different force-fields (AM1BCCv1/ZAP-9, AM1-BCCv1/Bondi, OPLS-AA, and PARSE) on the model performance. Our study provides useful insights on differential geometry-based implicit solvent models as well as improving the performance and robustness of these models.

欢迎大家参加！